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SUPPORTING INFORMATION

Searching for Missing Binary Equiatomic Phases: Complex Crystal Chemistry in the Hf–In System

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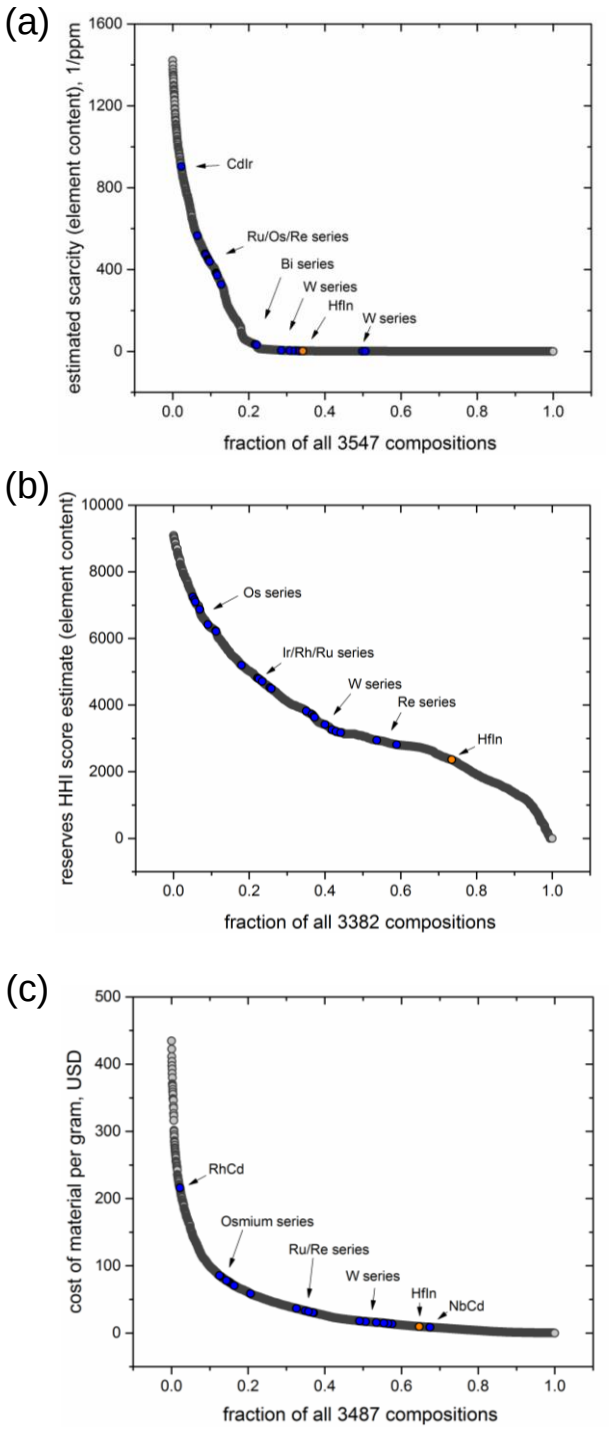


Figure S1. Estimated (a) scarcity, (b) HHI reserve score (excluding U- and Th-containing compounds), and (c) cost per gram (excluding Pm-containing compounds) for all possible *AB* combinations, with 21 uninvestigated systems highlighted. Calculations were made on the basis of a scarcity calculator and vendor internet prices.

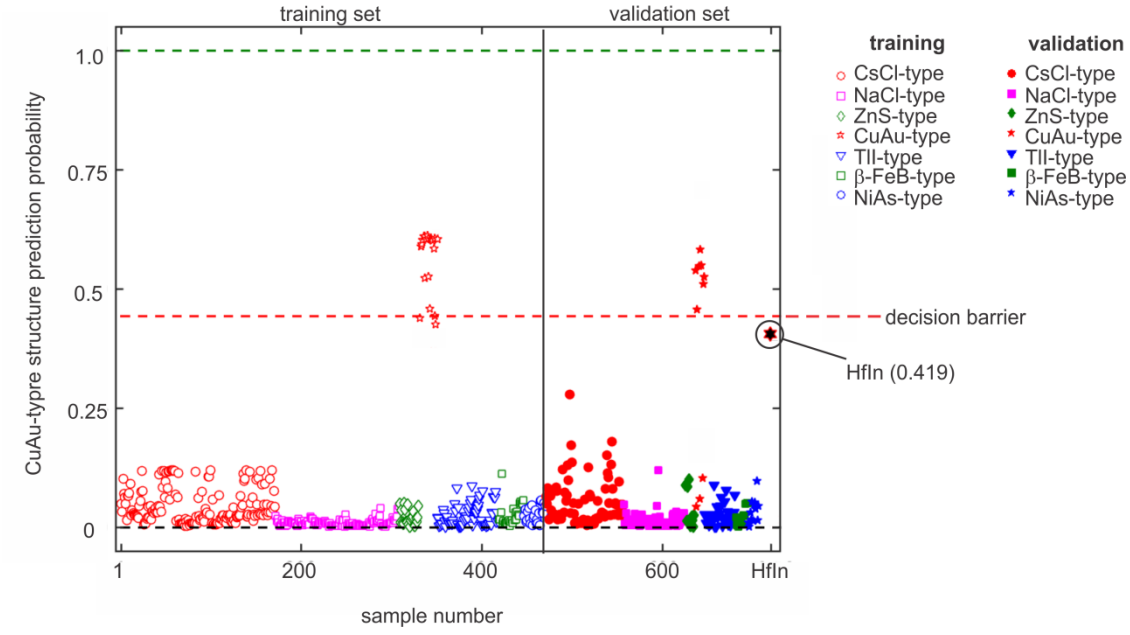
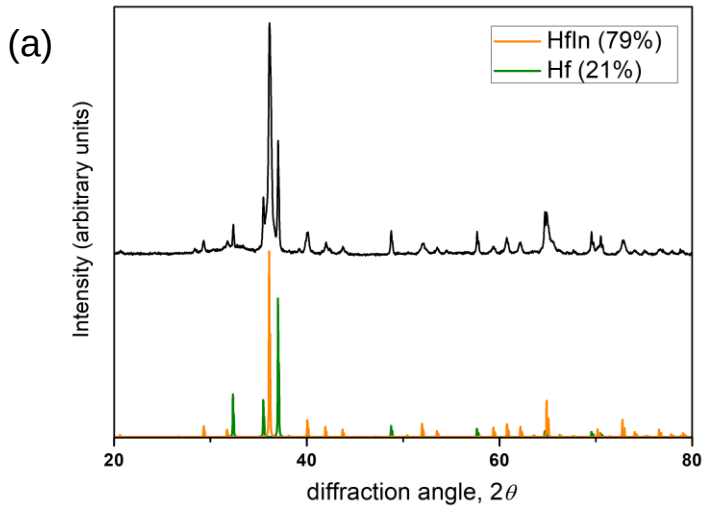


Figure S2. Probabilities predicted by machine-learning model to adopt CuAu-type structures for *AB* compounds, including HfIn.



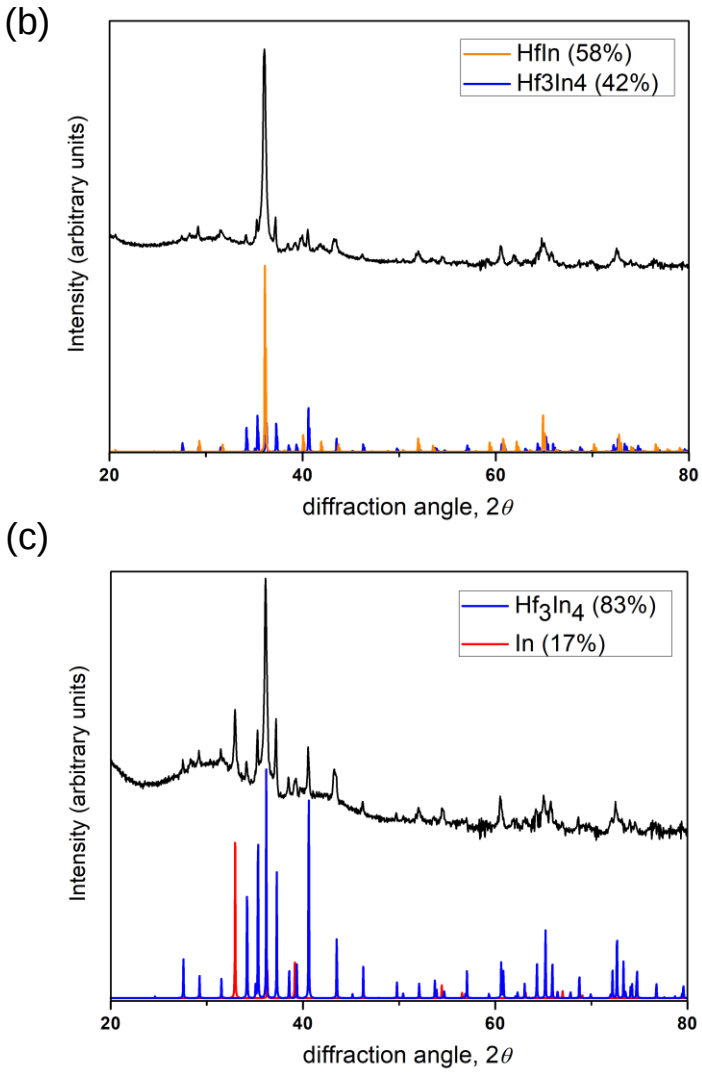
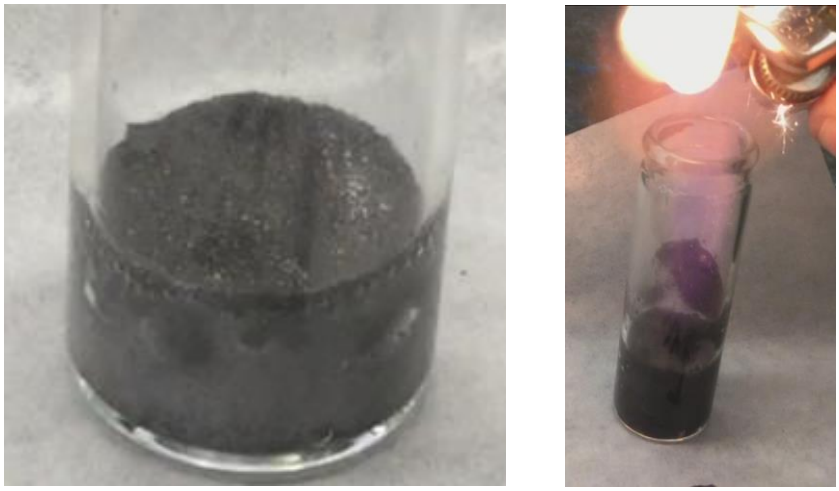


Figure S3. Powder XRD patterns for two-phase samples in Hf–In system.

(a)



(b)

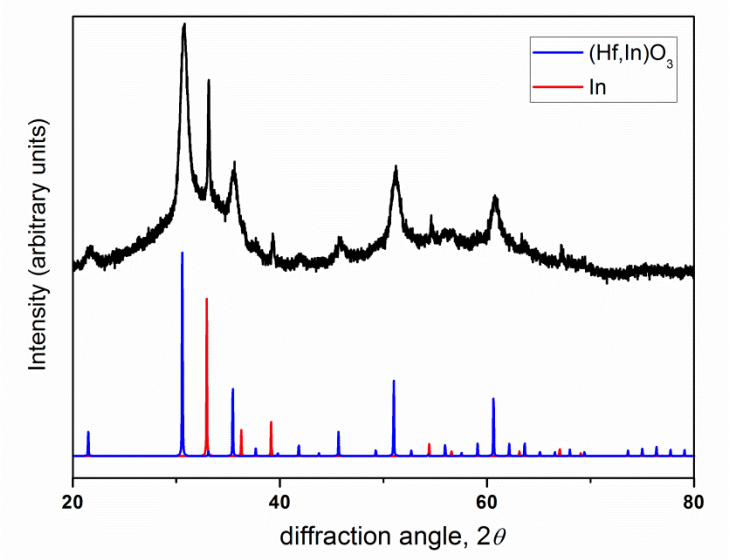


Figure S4. (a) Reaction of HfIn with water and ignition of flammable gas produced. (b) Powder XRD pattern of product after reaction with water.